



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 24, 2017 – 05:01 PM EST

PDB ID : 5M6U
Title : HUMAN PI3KDELTA IN COMPLEX WITH LASW1579
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Deposited on : 2016-10-26
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

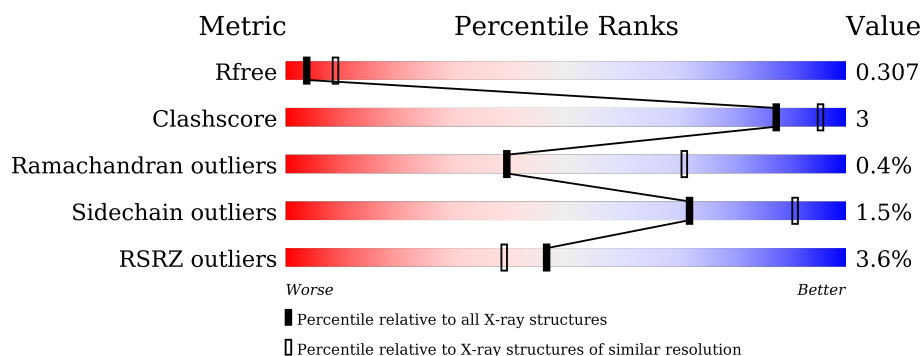
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

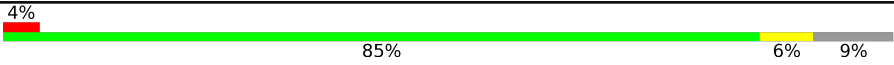

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1011	
2	B	724	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7700 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	916	Total	C	N	O	S	0	0	0
			6419	4072	1123	1179	45			

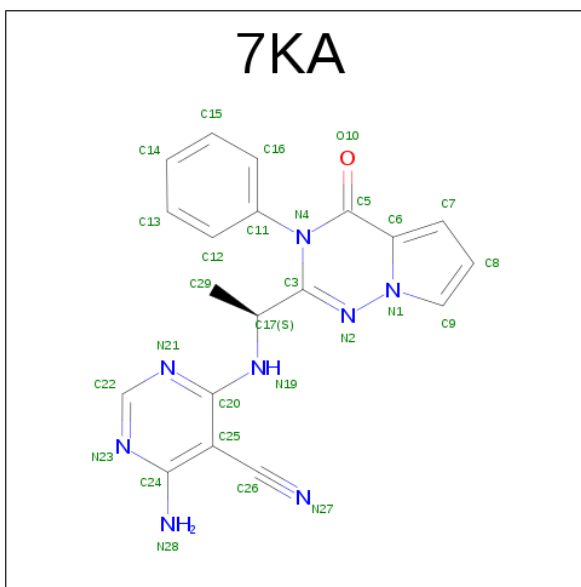
- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1253	795	210	244	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	469	ASP	GLU	conflict	UNP P27986
B	519	THR	LYS	conflict	UNP P27986
B	529	GLU	ASP	conflict	UNP P27986
B	539	VAL	ILE	conflict	UNP P27986

- Molecule 3 is 4-azanyl-6-[[1 {S}]-1-(4-oxidanylidene-3-phenyl-pyrrolo[2,1-f][1,2,4]triazin-2-yl)ethyl]amino]pyrimidine-5-carbonitrile (three-letter code: 7KA) (formula: C₁₉H₁₆N₈O).

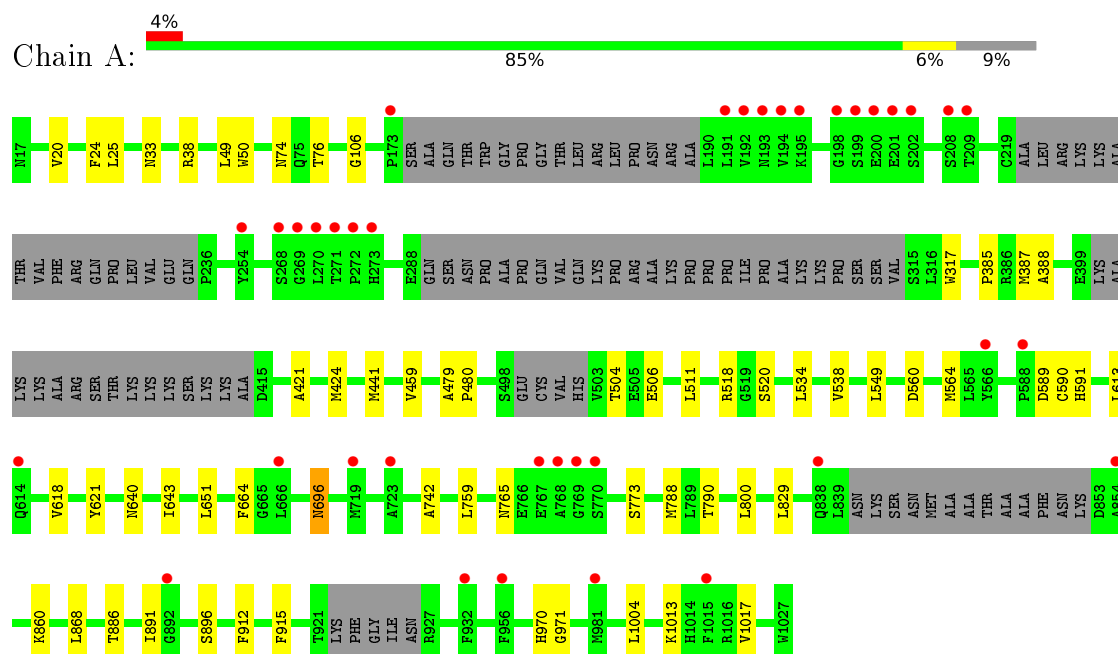


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	8	1		

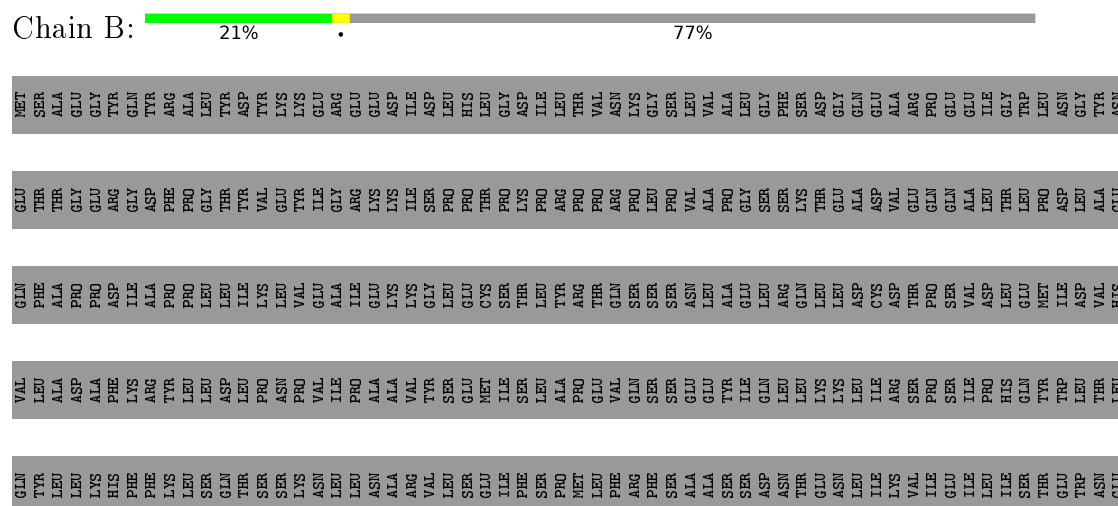
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



ILE	ASP	ASP	VAL	SER	ARG
ASN	ASP	GLU	LYS	THR	GLN
LYS	GLU	GLU	LYS	LYS	PRO
THR	ASP	LEU	LEU	MET	ALA
ALA	LEU	LEU	LEU	HIS	PRO
THR	PRO	THR	TYR	GLY	ALA
GLY	HIS	PRO	PRO	ASP	LEU
THR	HIS	VAL	VAL	TYR	PRO
PHY	ASP	SER	SER	THR	PRO
GLU	GLU	LYS	LYS	LEU	LYS
ALA	LYS	TYR	TYR	THR	PRO
GLU	THR	GLN	GLN	LEU	PRO
PRO	THR	GLN	ASP	ARG	LYS
TYR	ASN	ASP	GLN	GLY	THR
ASN	VAL	GLY	9436	ASN	VAL
THR	SER	SER	9439	ASN	VAL
SER	ASN	SER	1442	LYS	ALA
LEU	ARG	ARG	1442	LEU	ASN
LYS	ASN	LYS	9445	ILE	GLY
GLU	LYS	ALA	9445	ILE	MET
LEU	ALA	ALA	1449	ILE	ASN
VAL	GLU	GLU	1449	PHI	ASN
LEU	ASN	ASN	9455	HIS	ASN
HIS	LEU	LEU	9455	ARG	ASN
THR	LEU	THR	9455	ASP	MET
GLN	ARG	ARG	9474	GLY	SER
GLY	GLY	GLY	9481	LYS	LEU
HIS	GLY	LYS	9481	THR	GLN
SER	ARG	ARG	1486	GLY	ASP
VAL	GLY	GLY	1486	PHI	GLU
GLN	THR	THR	9497	SER	TRP
HIS	THR	THR	9497	ASP	TYR
ASN	LEU	PHI	9501	PRO	TRP
ASP	VAL	LEU	9501	LEU	GLY
SER	VAL	VAL	9528	THR	ASP
LEU	ARG	ARG	9528	PHI	ILE
ASN	GLU	GLU	9542	SER	SER
VAL	SER	SER	9542	VAL	ARG
THR	SER	SER	1549	VAL	GLU
LEU	LYS	LYS	1549	VAL	GLU
ALA	GLY	GLN	1584	GLU	VAL
TYR	CYS	GLY	1584	LEU	ASN
PRO	THR	THR	9589	ILE	GLU
VAL	ALA	VAL	9589	ASN	LYS
THR	CYS	CYS	9599	HIS	LEU
ALA	SER	THR	9599	TYR	ARG
GLN	VAL	ASN	ASN	ARG	ASP
GLN	VAL	VAL	GLU	ASN	THR
ARG	VAL	THR	THR	GLU	ALA
ARG	VAL	ASP	GLU	SER	GLY
		GLY	ASP	LEU	THR
		VAL	GLN	ALA	PHI
		VAL	TYR	THR	LEU
		VAL	SER	ASN	VAL
		HIS	LEU	PRO	ARG
		CYS	THR	LYS	ASP
		VAL	GLU	THR	ASP

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.49Å 113.21Å 144.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.08 – 2.85 48.28 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (89.08-2.85) 100.0 (48.28-2.85)	Depositor EDS
R_{merge}	4.00	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.256 , 0.309 0.250 , 0.307	Depositor DCC
R_{free} test set	997 reflections (2.84%)	DCC
Wilson B-factor (Å ²)	99.4	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 91.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7700	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7KA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/6560	0.57	0/8953
2	B	0.44	0/1272	0.59	1/1719 (0.1%)
All	All	0.43	0/7832	0.57	1/10672 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	542	ARG	NE-CZ-NH1	5.45	123.03	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6419	0	5292	31	0
2	B	1253	0	1064	6	0
3	A	28	0	0	0	0
All	All	7700	0	6356	36	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 36 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:ALA:HB3	1:A:765:ASN:HB3	1.72	0.71
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.86	0.58
1:A:25:LEU:HD13	2:B:497:GLN:HG3	1.88	0.56
1:A:971:GLY:HA3	1:A:1004:LEU:HD21	1.92	0.51
1:A:613:LEU:HD13	1:A:788:MET:HE1	1.93	0.50

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	900/1011 (89%)	850 (94%)	46 (5%)	4 (0%)	39	71
2	B	162/724 (22%)	157 (97%)	5 (3%)	0	100	100
All	All	1062/1735 (61%)	1007 (95%)	51 (5%)	4 (0%)	39	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	ARG
1	A	520	SER
1	A	106	GLY
1	A	896	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/896 (55%)	486 (99%)	7 (1%)	74	91
2	B	98/654 (15%)	96 (98%)	2 (2%)	63	87
All	All	591/1550 (38%)	582 (98%)	9 (2%)	72	91

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	560	ASP
2	B	501	GLN
1	A	915	PHE
1	A	317	TRP
1	A	696	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	614	GLN
1	A	944	GLN
1	A	792	GLN
1	A	193	ASN
1	A	918	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	7KA	A	1101	-	28,31,31	1.25	3 (10%)	23,44,44	1.75	5 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7KA	A	1101	-	-	0/8/14/14	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	7KA	C11-N4	-4.11	1.40	1.46
3	A	1101	7KA	C20-N19	2.63	1.39	1.35
3	A	1101	7KA	C5-C6	2.82	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	7KA	N21-C22-N23	-3.83	122.05	128.65
3	A	1101	7KA	C25-C20-N21	-3.43	118.02	121.23
3	A	1101	7KA	C12-C11-N4	2.29	122.10	119.25
3	A	1101	7KA	C20-C25-C26	3.28	123.81	119.35
3	A	1101	7KA	C8-C9-N1	3.68	109.05	106.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	916/1011 (90%)	0.11	37 (4%) 42 34	64, 108, 177, 227	0
2	B	164/724 (22%)	-0.19	2 (1%) 81 78	71, 91, 120, 143	0
All	All	1080/1735 (62%)	0.06	39 (3%) 46 39	64, 103, 174, 227	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	GLU	9.5
1	A	202	SER	8.9
1	A	268	SER	8.6
1	A	201	GLU	6.9
1	A	269	GLY	5.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	7KA	A	1101	28/28	0.94	0.21	0.45	68,98,106,107	0

6.5 Other polymers ⓘ

There are no such residues in this entry.